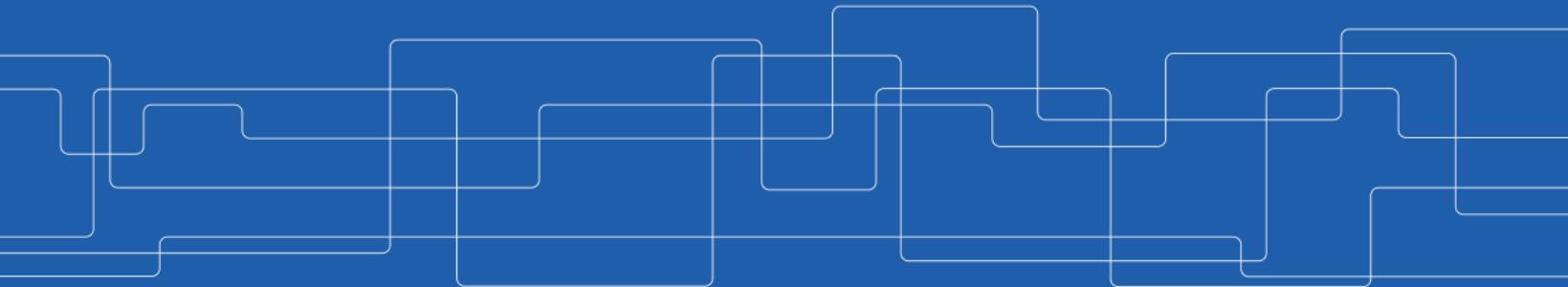




Machine Learning - Regressions

Amir H. Payberah
payberah@kth.se
07/11/2018



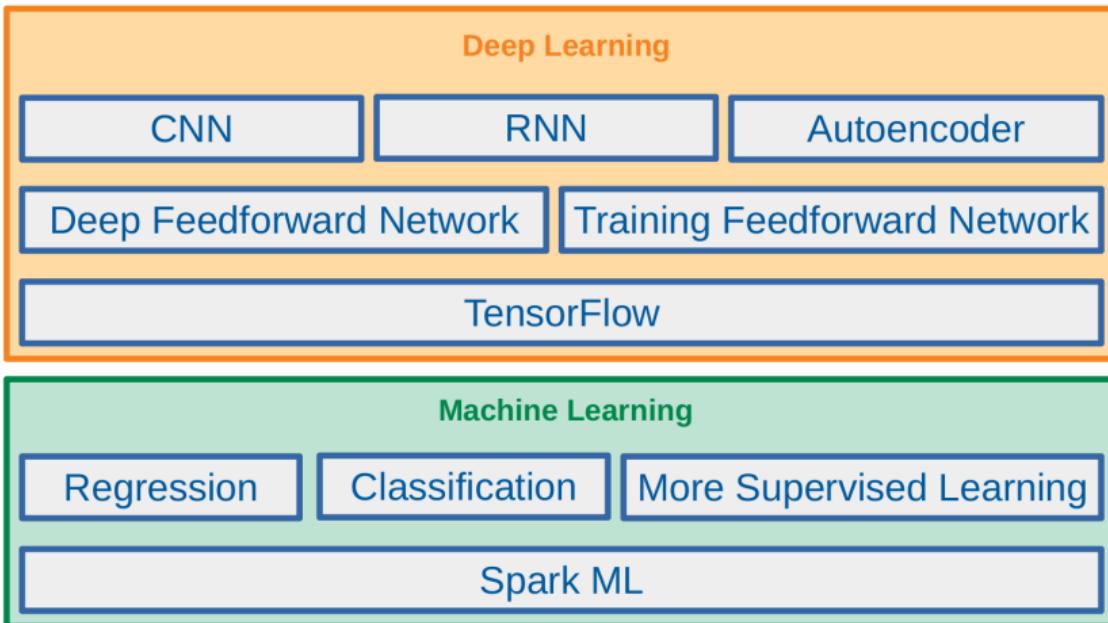


The Course Web Page

<https://id2223kth.github.io>

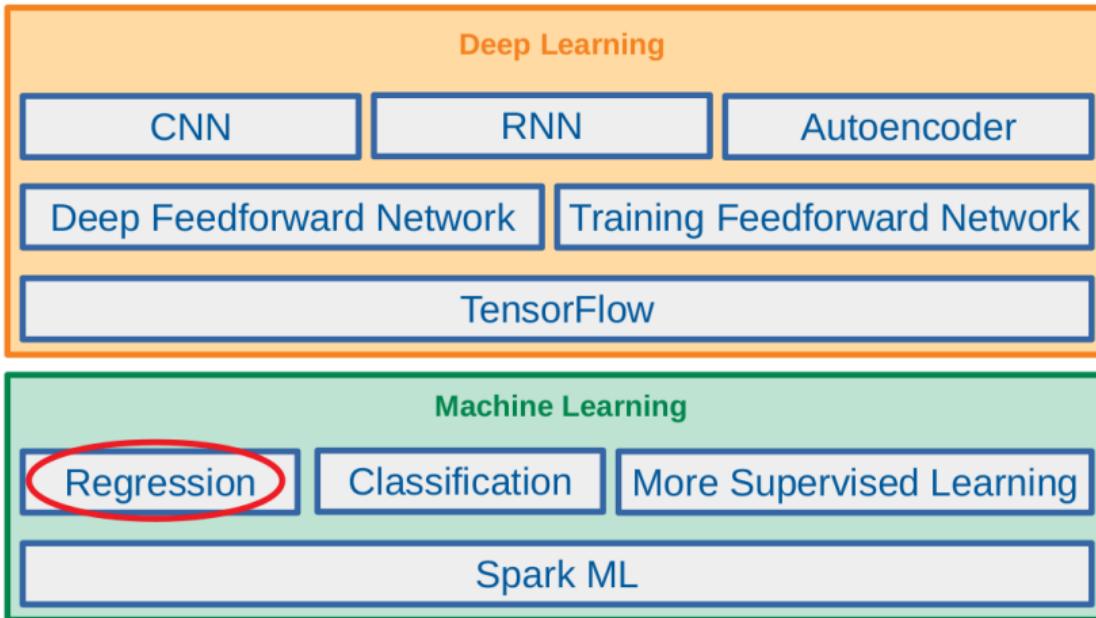


Where Are We?





Where Are We?





Let's Start with an Example



The Housing Price Example (1/3)

- ▶ Given the dataset of m houses.

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:



The Housing Price Example (1/3)

- Given the dataset of m houses.

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:

- Predict the prices of other houses, as a function of the size of living area and number of bedrooms?



The Housing Price Example (2/3)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:
:	:	:



The Housing Price Example (2/3)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:

$$\mathbf{x}^{(1)} = \begin{bmatrix} 2104 \\ 3 \end{bmatrix} \quad y^{(1)} = 400 \quad \mathbf{x}^{(2)} = \begin{bmatrix} 1600 \\ 3 \end{bmatrix} \quad y^{(2)} = 330 \quad \mathbf{x}^{(3)} = \begin{bmatrix} 2400 \\ 3 \end{bmatrix} \quad y^{(3)} = 369$$

The Housing Price Example (2/3)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:

$$\mathbf{x}^{(1)} = \begin{bmatrix} 2104 \\ 3 \end{bmatrix} \quad y^{(1)} = 400 \quad \mathbf{x}^{(2)} = \begin{bmatrix} 1600 \\ 3 \end{bmatrix} \quad y^{(2)} = 330 \quad \mathbf{x}^{(3)} = \begin{bmatrix} 2400 \\ 3 \end{bmatrix} \quad y^{(3)} = 369$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \mathbf{x}^{(3)\top} \\ \vdots \end{bmatrix} = \begin{bmatrix} 2104 & 3 \\ 1600 & 3 \\ 2400 & 3 \\ \vdots & \vdots \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ \vdots \end{bmatrix}$$

The Housing Price Example (2/3)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:

$$\mathbf{x}^{(1)} = \begin{bmatrix} 2104 \\ 3 \end{bmatrix} \quad y^{(1)} = 400 \quad \mathbf{x}^{(2)} = \begin{bmatrix} 1600 \\ 3 \end{bmatrix} \quad y^{(2)} = 330 \quad \mathbf{x}^{(3)} = \begin{bmatrix} 2400 \\ 3 \end{bmatrix} \quad y^{(3)} = 369$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \mathbf{x}^{(3)\top} \\ \vdots \end{bmatrix} = \begin{bmatrix} 2104 & 3 \\ 1600 & 3 \\ 2400 & 3 \\ \vdots & \vdots \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ \vdots \end{bmatrix}$$

- $\mathbf{x}^{(i)} \in \mathbb{R}^2$: $x_1^{(i)}$ is the living area, and $x_2^{(i)}$ is the number of bedrooms of the i th house in the training set.

The Housing Price Example (3/3)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:

- ▶ Predict the prices of other houses \hat{y} as a function of the size of their living areas x_1 , and number of bedrooms x_2 , i.e., $\hat{y} = f(x_1, x_2)$
- ▶ E.g., what is \hat{y} , if $x_1 = 4000$ and $x_2 = 4$?

The Housing Price Example (3/3)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
:	:	:

- ▶ Predict the prices of other houses \hat{y} as a function of the size of their living areas x_1 , and number of bedrooms x_2 , i.e., $\hat{y} = f(x_1, x_2)$
- ▶ E.g., what is \hat{y} , if $x_1 = 4000$ and $x_2 = 4$?
- ▶ As an initial choice: $\hat{y} = f_w(\mathbf{x}) = w_1x_1 + w_2x_2$



Linear Regression



Linear Regression (1/2)

- Our goal: to build a system that takes input $\mathbf{x} \in \mathbb{R}^n$ and predicts output $\hat{\mathbf{y}} \in \mathbb{R}$.



Linear Regression (1/2)

- ▶ Our goal: to build a system that takes input $\mathbf{x} \in \mathbb{R}^n$ and predicts output $\hat{y} \in \mathbb{R}$.
- ▶ In linear regression, the output \hat{y} is a linear function of the input \mathbf{x} .

$$\hat{y} = f_w(\mathbf{x}) = w_1x_1 + w_2x_2 + \cdots + w_nx_n$$

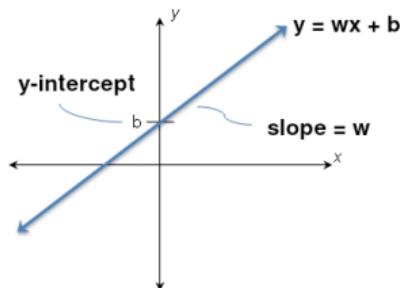
$$\hat{y} = \mathbf{w}^\top \mathbf{x}$$

- \hat{y} : the predicted value
- n : the number of features
- x_i : the i th feature value
- w_j : the j th model parameter ($\mathbf{w} \in \mathbb{R}^n$)

Linear Regression (2/2)

- ▶ Linear regression often has one additional parameter, called **intercept b**:

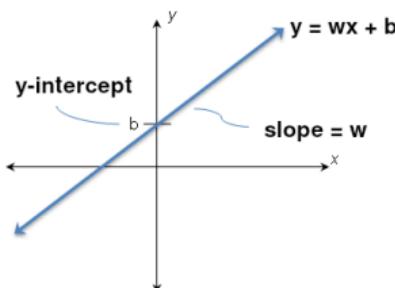
$$\hat{y} = \mathbf{w}^T \mathbf{x} + b$$



Linear Regression (2/2)

- ▶ Linear regression often has one additional parameter, called **intercept** b :

$$\hat{y} = \mathbf{w}^T \mathbf{x} + b$$



- ▶ Instead of adding the bias parameter b , we can augment \mathbf{x} with an **extra entry** that is **always set to 1**.

$$\hat{y} = f_w(\mathbf{x}) = w_0 x_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n, \text{ where } x_0 = 1$$



Linear Regression - Model Parameters

- ▶ Parameters $w \in \mathbb{R}^n$ are values that control the behavior of the system.



Linear Regression - Model Parameters

- ▶ Parameters $w \in \mathbb{R}^n$ are values that control the behavior of the system.
- ▶ w are a set of weights that determine how each feature affects the prediction.



Linear Regression - Model Parameters

- ▶ Parameters $w \in \mathbb{R}^n$ are values that **control the behavior of the system**.
- ▶ w are a set of **weights** that determine how each **feature affects the prediction**.
 - $w_i > 0$: increasing the value of the feature x_i , increases the value of our prediction \hat{y} .



Linear Regression - Model Parameters

- ▶ Parameters $w \in \mathbb{R}^n$ are values that control the behavior of the system.
- ▶ w are a set of weights that determine how each feature affects the prediction.
 - $w_i > 0$: increasing the value of the feature x_i , increases the value of our prediction \hat{y} .
 - $w_i < 0$: increasing the value of the feature x_i , decreases the value of our prediction \hat{y} .



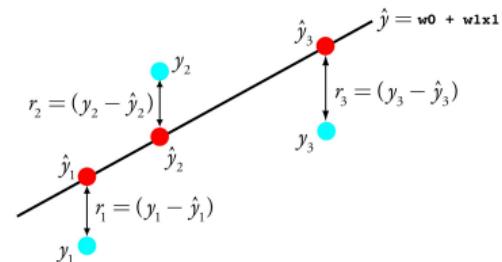
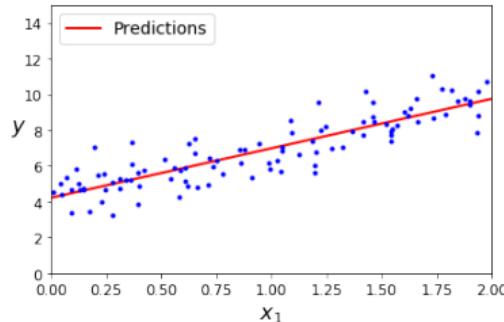
Linear Regression - Model Parameters

- ▶ Parameters $w \in \mathbb{R}^n$ are values that **control the behavior of the system**.
- ▶ w are a set of **weights** that determine how each **feature affects the prediction**.
 - $w_i > 0$: increasing the value of the feature x_i , increases the value of our prediction \hat{y} .
 - $w_i < 0$: increasing the value of the feature x_i , decreases the value of our prediction \hat{y} .
 - $w_i = 0$: the value of the feature x_i , has no effect on the prediction \hat{y} .



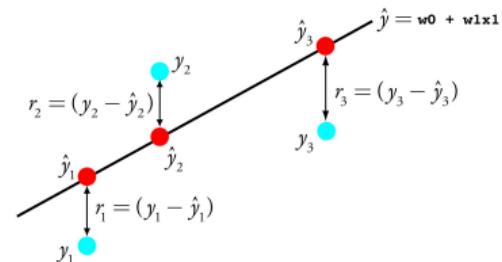
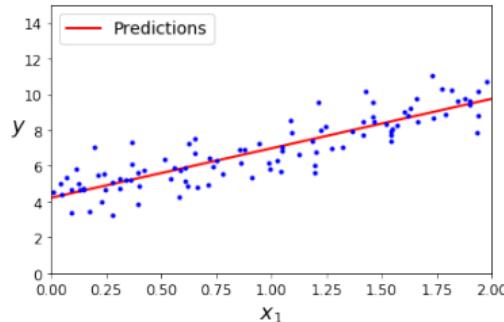
How to Learn Model Parameters w ?

Linear Regression - Cost Function (1/2)



- One reasonable model should make \hat{y} close to y , at least for the training dataset.

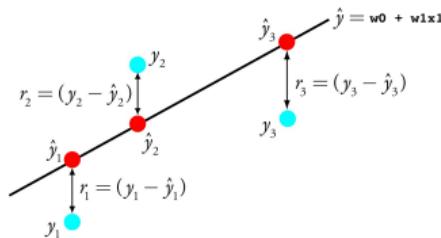
Linear Regression - Cost Function (1/2)



- One reasonable model should make \hat{y} close to y , at least for the training dataset.
- Residual: the difference between the dependent variable y and the predicted value \hat{y} .

$$r^{(i)} = y^{(i)} - \hat{y}^{(i)}$$

Linear Regression - Cost Function (2/2)

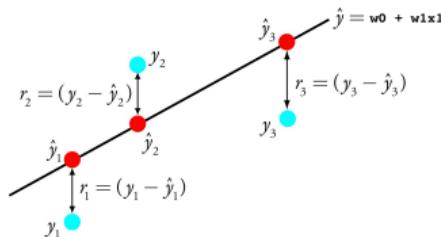


► Cost function $J(\mathbf{w})$

- For each value of the \mathbf{w} , it measures how close the $\hat{y}^{(i)}$ is to the corresponding $y^{(i)}$.
- We can define $J(\mathbf{w})$ as the mean squared error (MSE):

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^m (\hat{y}^{(i)} - y^{(i)})^2$$

Linear Regression - Cost Function (2/2)



► Cost function $J(\mathbf{w})$

- For each value of the \mathbf{w} , it measures how **close** the $\hat{y}^{(i)}$ is to the corresponding $y^{(i)}$.
- We can define $J(\mathbf{w})$ as the **mean squared error (MSE)**:

$$\begin{aligned} J(\mathbf{w}) &= \text{MSE}(\mathbf{w}) = \frac{1}{m} \sum_{i}^m (\hat{y}^{(i)} - y^{(i)})^2 \\ &= E[(\hat{y} - y)^2] = \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 \end{aligned}$$



How to Learn Model Parameters?

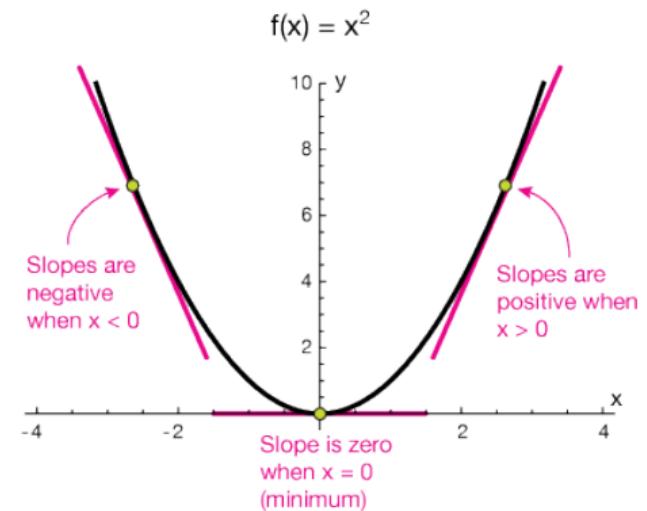
- ▶ We want to choose \mathbf{w} so as to minimize $J(\mathbf{w})$.
- ▶ Two approaches to find \mathbf{w} :
 - Normal equation
 - Gradient descent



Normal Equation

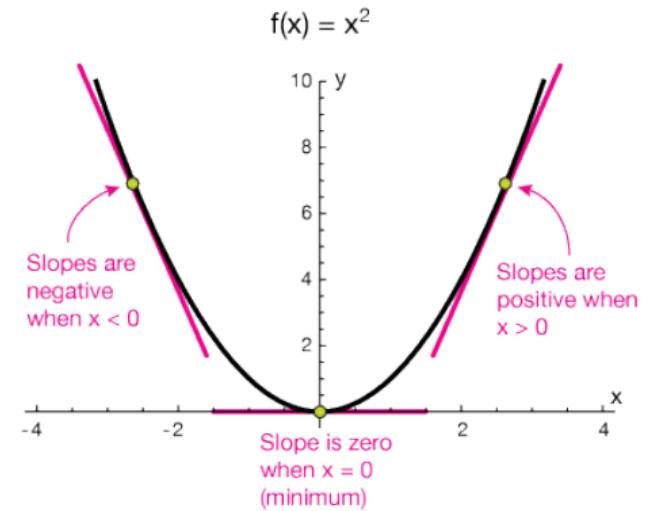
Derivatives and Gradient (1/3)

- The **first derivative** of $f(x)$, shown as $f'(x)$, shows the **slope** of the **tangent line** to the function at the point x .



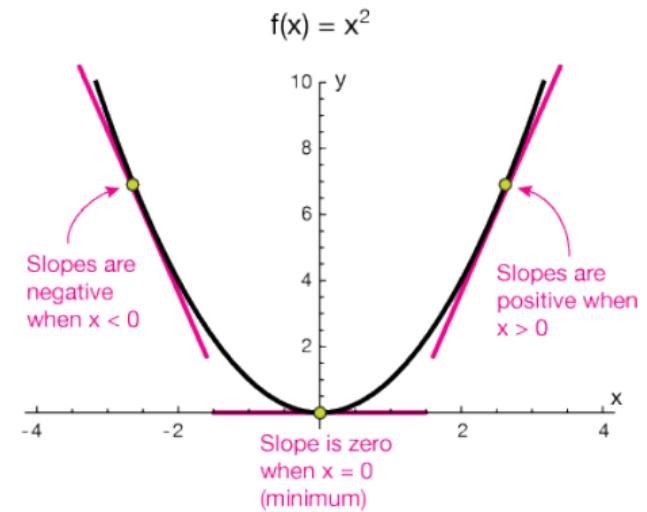
Derivatives and Gradient (1/3)

- ▶ The **first derivative** of $f(x)$, shown as $f'(x)$, shows the **slope** of the **tangent line** to the **function** at the point x .
- ▶ $f(x) = x^2 \Rightarrow f'(x) = 2x$



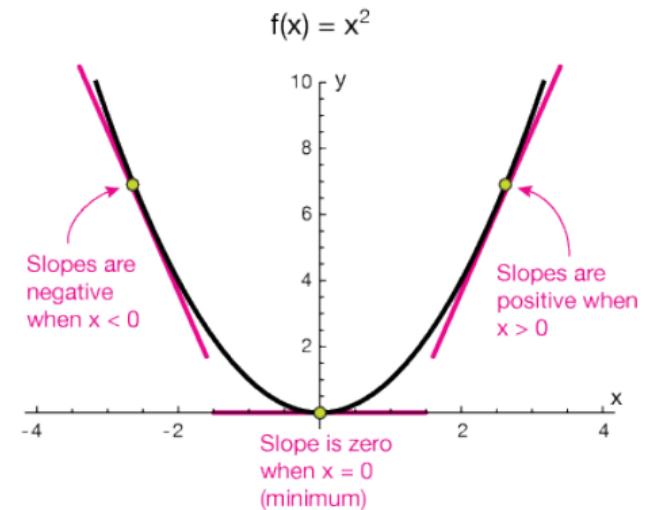
Derivatives and Gradient (1/3)

- ▶ The **first derivative** of $f(x)$, shown as $f'(x)$, shows the **slope** of the **tangent line** to the **function** at the point x .
- ▶ $f(x) = x^2 \Rightarrow f'(x) = 2x$
- ▶ If $f(x)$ is increasing, then $f'(x) > 0$



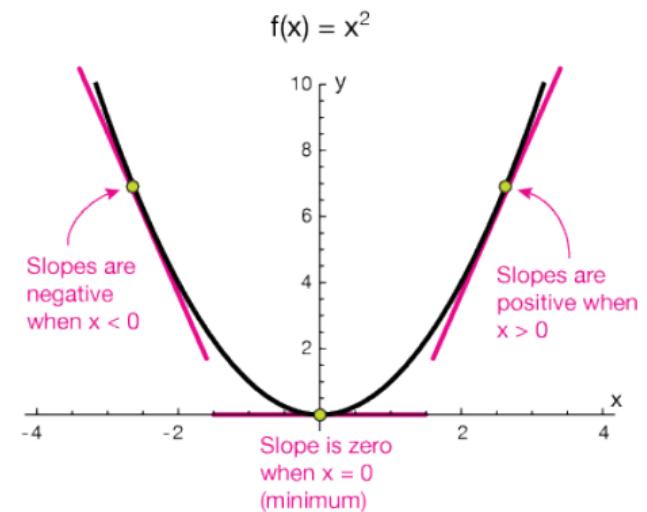
Derivatives and Gradient (1/3)

- ▶ The **first derivative** of $f(x)$, shown as $f'(x)$, shows the **slope** of the **tangent line** to the **function** at the point x .
- ▶ $f(x) = x^2 \Rightarrow f'(x) = 2x$
- ▶ If $f(x)$ is **increasing**, then $f'(x) > 0$
- ▶ If $f(x)$ is **decreasing**, then $f'(x) < 0$



Derivatives and Gradient (1/3)

- ▶ The **first derivative** of $f(x)$, shown as $f'(x)$, shows the **slope** of the **tangent line** to the **function** at the point x .
- ▶ $f(x) = x^2 \Rightarrow f'(x) = 2x$
- ▶ If $f(x)$ is **increasing**, then $f'(x) > 0$
- ▶ If $f(x)$ is **decreasing**, then $f'(x) < 0$
- ▶ If $f(x)$ is at local **minimum/maximum**, then $f'(x) = 0$





Derivatives and Gradient (2/3)

- ▶ What if a function has multiple arguments, e.g., $f(x_1, x_2, \dots, x_n)$
- ▶ **Partial derivatives:** the derivative with respect to a **particular argument**.
 - $\frac{\partial f}{\partial x_1}$, the derivative **with respect to x_1**
 - $\frac{\partial f}{\partial x_2}$, the derivative **with respect to x_2**



Derivatives and Gradient (2/3)

- ▶ What if a function has multiple arguments, e.g., $f(x_1, x_2, \dots, x_n)$
- ▶ **Partial derivatives:** the derivative with respect to a particular argument.
 - $\frac{\partial f}{\partial x_1}$, the derivative with respect to x_1
 - $\frac{\partial f}{\partial x_2}$, the derivative with respect to x_2
- ▶ $\frac{\partial f}{\partial x_i}$: shows how much the function f will change, if we change x_i .

Derivatives and Gradient (2/3)

- ▶ What if a function has multiple arguments, e.g., $f(x_1, x_2, \dots, x_n)$
- ▶ **Partial derivatives:** the derivative with respect to a particular argument.
 - $\frac{\partial f}{\partial x_1}$, the derivative with respect to x_1
 - $\frac{\partial f}{\partial x_2}$, the derivative with respect to x_2
- ▶ $\frac{\partial f}{\partial x_i}$: shows how much the function f will change, if we change x_i .
- ▶ **Gradient:** the vector of all partial derivatives for a function f .

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$



Derivatives and Gradient (3/3)

- ▶ What is the gradient of $f(x_1, x_2, x_3) = x_1 - x_1x_2 + x_3^2$?

Derivatives and Gradient (3/3)

- ▶ What is the gradient of $f(x_1, x_2, x_3) = x_1 - x_1x_2 + x_3^2$?

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial}{\partial x_1}(x_1 - x_1x_2 + x_3^2) \\ \frac{\partial}{\partial x_2}(x_1 - x_1x_2 + x_3^2) \\ \frac{\partial}{\partial x_3}(x_1 - x_1x_2 + x_3^2) \end{bmatrix} = \begin{bmatrix} 1 - x_2 \\ -x_1 \\ 2x_3 \end{bmatrix}$$



Normal Equation (1/2)

- ▶ To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$\hat{y} = \mathbf{w}^T \mathbf{x}$$



Normal Equation (1/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$\hat{\mathbf{y}} = \mathbf{w}^T \mathbf{x}$$

$$\mathbf{X} = \begin{bmatrix} [x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(1)}] \\ [x_1^{(2)}, x_2^{(2)}, \dots, x_n^{(2)}] \\ \vdots \\ [x_1^{(m)}, x_2^{(m)}, \dots, x_n^{(m)}] \end{bmatrix} = \begin{bmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \vdots \\ \mathbf{x}^{(m)\top} \end{bmatrix} \quad \hat{\mathbf{y}} = \begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix}$$

Normal Equation (1/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$\hat{\mathbf{y}} = \mathbf{w}^T \mathbf{x}$$

$$\mathbf{X} = \begin{bmatrix} [x_1^{(1)}, x_2^{(1)}, \dots, x_n^{(1)}] \\ [x_1^{(2)}, x_2^{(2)}, \dots, x_n^{(2)}] \\ \vdots \\ [x_1^{(m)}, x_2^{(m)}, \dots, x_n^{(m)}] \end{bmatrix} = \begin{bmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \vdots \\ \mathbf{x}^{(m)\top} \end{bmatrix} \quad \hat{\mathbf{y}} = \begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix}$$

$$\hat{\mathbf{y}} = \mathbf{w}^T \mathbf{X}^\top \text{ or } \hat{\mathbf{y}} = \mathbf{X} \mathbf{w}$$



Normal Equation (2/2)

- ▶ To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$



Normal Equation (2/2)

- ▶ To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$J(\mathbf{w}) = \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2, \nabla_{\mathbf{w}} J(\mathbf{w}) = 0$$

Normal Equation (2/2)

- ▶ To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$\begin{aligned}J(\mathbf{w}) &= \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2, \quad \nabla_{\mathbf{w}} J(\mathbf{w}) = 0 \\&\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 = 0\end{aligned}$$

Normal Equation (2/2)

- ▶ To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$J(\mathbf{w}) = \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2, \nabla_{\mathbf{w}} J(\mathbf{w}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\mathbf{Xw} - \mathbf{y}\|_2^2 = 0$$

Normal Equation (2/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$\begin{aligned}J(\mathbf{w}) &= \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2, \quad \nabla_{\mathbf{w}} J(\mathbf{w}) = 0 \\&\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 = 0 \\&\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 = 0 \\&\Rightarrow \nabla_{\mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) = 0\end{aligned}$$

Normal Equation (2/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$J(\mathbf{w}) = \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2, \nabla_{\mathbf{w}} J(\mathbf{w}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{y} + \mathbf{y}^\top \mathbf{y}) = 0$$

Normal Equation (2/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$J(\mathbf{w}) = \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2, \nabla_{\mathbf{w}} J(\mathbf{w}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{y} + \mathbf{y}^\top \mathbf{y}) = 0$$

$$\Rightarrow 2\mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{X}^\top \mathbf{y} = 0$$

Normal Equation (2/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$J(\mathbf{w}) = \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2, \nabla_{\mathbf{w}} J(\mathbf{w}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\hat{\mathbf{y}} - \mathbf{y}\|_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w} - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{y} + \mathbf{y}^\top \mathbf{y}) = 0$$

$$\Rightarrow 2\mathbf{X}^\top \mathbf{X} \mathbf{w} - 2\mathbf{X}^\top \mathbf{y} = 0$$

$$\Rightarrow \mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Normal Equation - Example (1/7)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540

- ▶ Predict the value of \hat{y} , when $x_1 = 4000$ and $x_2 = 4$.

Normal Equation - Example (1/7)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540

- ▶ Predict the value of \hat{y} , when $x_1 = 4000$ and $x_2 = 4$.
- ▶ We should find w_0 , w_1 , and w_2 in $\hat{y} = w_0 + w_1x_1 + w_2x_2$.
- ▶ $w = (X^T X)^{-1} X^T y$.



Normal Equation - Example (2/7)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540

$$\mathbf{X} = \begin{bmatrix} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

```
import breeze.linalg._

val X = new DenseMatrix(5, 3, Array(1.0, 1.0, 1.0, 1.0, 1.0,
                                         2104.0, 1600.0, 2400.0, 1416.0, 3000.0,
                                         3.0, 3.0, 3.0, 2.0, 4.0))
val y = new DenseVector(Array(400.0, 330.0, 369.0, 232.0, 540.0))
```

Normal Equation - Example (3/7)

$$\mathbf{X}^T \mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 2104 & 1600 & 2400 & 1416 & 3000 \\ 3 & 3 & 3 & 2 & 4 \end{bmatrix} \begin{bmatrix} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{bmatrix} = \begin{bmatrix} 5 & 10520 & 10520 \\ 15 & 23751872 & 33144 \\ 15 & 33144 & 47 \end{bmatrix}$$

```
val Xt = X.t  
val XtX = Xt * X
```



Normal Equation - Example (4/7)

$$(\mathbf{X}^T \mathbf{X})^{-1} = \begin{bmatrix} 4.90366455e + 00 & 7.48766737e - 04 & -2.09302326e + 00 \\ 7.48766737e - 04 & 2.75281889e - 06 & -2.18023256e - 03 \\ -2.09302326e + 00 & -2.18023256e - 03 & 2.22674419e + 00 \end{bmatrix}$$

```
val XtXInv = inv(XtX)
```



Normal Equation - Example (5/7)

$$\mathbf{X}^T \mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 2104 & 1600 & 2400 & 1416 & 3000 \\ 3 & 3 & 3 & 2 & 4 \end{bmatrix} \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix} = \begin{bmatrix} 1871 \\ 4203712 \\ 5921 \end{bmatrix}$$

```
val Xty = Xt * y
```



Normal Equation - Example (6/7)

$$\begin{aligned} \mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} &= \begin{bmatrix} 4.90366455e + 00 & 7.48766737e - 04 & -2.09302326e + 00 \\ 7.48766737e - 04 & 2.75281889e - 06 & -2.18023256e - 03 \\ -2.09302326e + 00 & -2.18023256e - 03 & 2.22674419e + 00 \end{bmatrix} \begin{bmatrix} 1871 \\ 4203712 \\ 5921 \end{bmatrix} \\ &= \begin{bmatrix} -7.04346018e + 01 \\ 6.38433756e - 02 \\ 1.03436047e + 02 \end{bmatrix} \end{aligned}$$

```
val w = XtxInv * Xty
```



Normal Equation - Example (7/7)

- ▶ Predict the value of y , when $x_1 = 4000$ and $x_2 = 4$.

$$\hat{y} = -7.04346018e + 01 + 6.38433756e - 02 \times 4000 + 1.03436047e + 02 \times 4 \approx 599$$

```
val test = new DenseVector(Array(1.0, 4000.0, 4.0))

val yHat = w * test
```



Normal Equation in Spark

```
case class house(x1: Long, x2: Long, y: Long)

val trainData = Seq(house(2104, 3, 400), house(1600, 3, 330), house(2400, 3, 369),
                    house(1416, 2, 232), house(3000, 4, 540)).toDF

val testData = Seq(house(4000, 4, 0)).toDF
```



Normal Equation in Spark

```
case class house(x1: Long, x2: Long, y: Long)

val trainData = Seq(house(2104, 3, 400), house(1600, 3, 330), house(2400, 3, 369),
                    house(1416, 2, 232), house(3000, 4, 540)).toDF

val testData = Seq(house(4000, 4, 0)).toDF
```

```
import org.apache.spark.ml.feature.VectorAssembler

val va = new VectorAssembler().setInputCols(Array("x1", "x2")).setOutputCol("features")

val train = va.transform(trainData)
val test = va.transform(testData)
```



Normal Equation in Spark

```
case class house(x1: Long, x2: Long, y: Long)

val trainData = Seq(house(2104, 3, 400), house(1600, 3, 330), house(2400, 3, 369),
                    house(1416, 2, 232), house(3000, 4, 540)).toDF

val testData = Seq(house(4000, 4, 0)).toDF
```

```
import org.apache.spark.ml.feature.VectorAssembler

val va = new VectorAssembler().setInputCols(Array("x1", "x2")).setOutputCol("features")

val train = va.transform(trainData)
val test = va.transform(testData)
```

```
import org.apache.spark.ml.regression.LinearRegression

val lr = new LinearRegression().setFeaturesCol("features").setLabelCol("y").setSolver("normal")
val lrModel = lr.fit(train)
lrModel.transform(test).show
```



Normal Equation - Computational Complexity

- ▶ The computational complexity of inverting $\mathbf{X}^T \mathbf{X}$ is $O(n^3)$.
 - For an $m \times n$ matrix (where n is the number of features).



Normal Equation - Computational Complexity

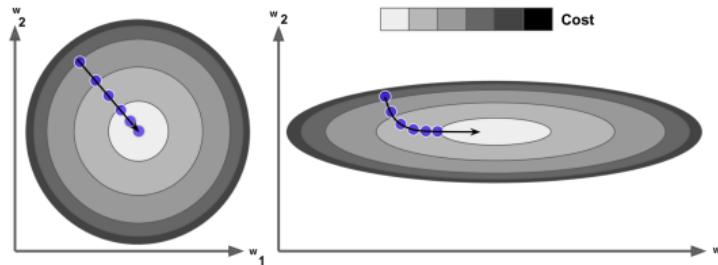
- ▶ The computational complexity of inverting $\mathbf{X}^T \mathbf{X}$ is $O(n^3)$.
 - For an $m \times n$ matrix (where n is the number of features).
- ▶ But, this equation is linear with regards to the number of instances in the training set (it is $O(m)$).
 - It handles large training sets efficiently, provided they can fit in memory.



Gradient Descent

Gradient Descent (1/2)

- ▶ Gradient descent is a generic optimization algorithm capable of finding optimal solutions to a wide range of problems.
- ▶ The idea: to tweak parameters iteratively in order to minimize a cost function.



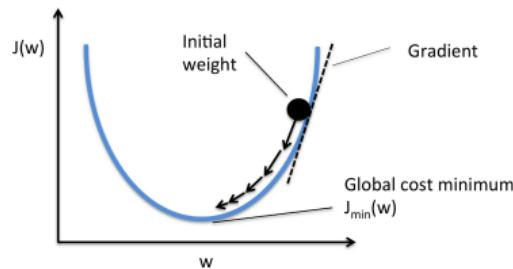
Gradient Descent (2/2)

- ▶ Suppose you are **lost** in the **mountains** in a dense fog.
- ▶ You can only feel the **slope** of the ground below your feet.
- ▶ A strategy to **get to the bottom** of the valley is to **go downhill** in the **direction of the steepest slope**.



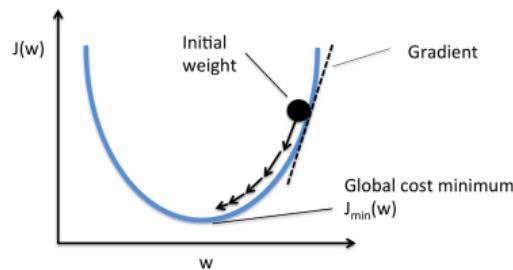
Gradient Descent - Iterative Optimization Algorithm

- ▶ Choose a starting point, e.g., filling w with random values.



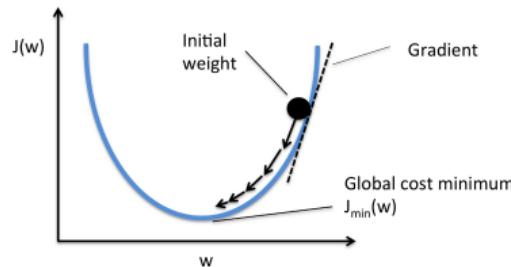
Gradient Descent - Iterative Optimization Algorithm

- ▶ Choose a starting point, e.g., filling w with random values.
- ▶ If the stopping criterion is true return the current solution, otherwise continue.



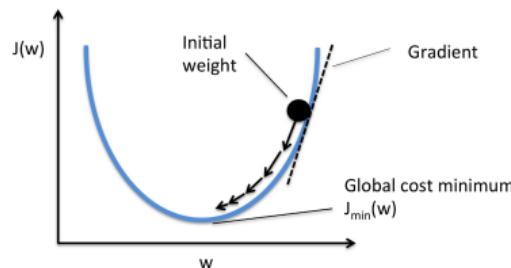
Gradient Descent - Iterative Optimization Algorithm

- ▶ Choose a **starting point**, e.g., filling \mathbf{w} with **random values**.
- ▶ If the **stopping criterion** is true return the **current solution**, otherwise continue.
- ▶ Find a **descent direction**, a **direction in which the function value decreases** near the current point.



Gradient Descent - Iterative Optimization Algorithm

- ▶ Choose a **starting point**, e.g., filling **w** with **random values**.
- ▶ If the **stopping criterion** is true return the **current solution**, otherwise continue.
- ▶ Find a **descent direction**, a **direction in which the function value decreases** near the current point.
- ▶ Determine the **step size**, the **length of a step** in the given direction.





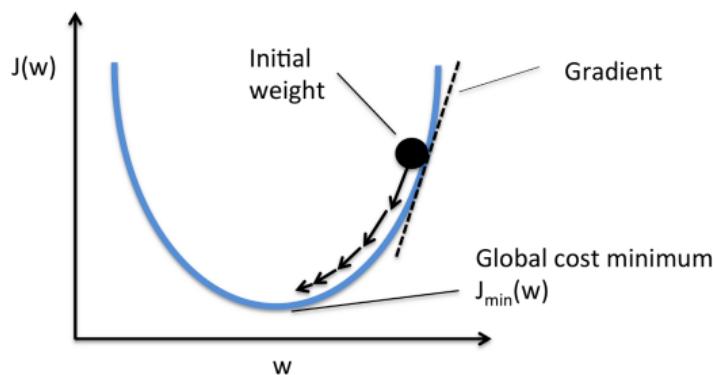
Gradient Descent - Key Points

- ▶ Stopping criterion
- ▶ Descent direction
- ▶ Step size (learning rate)

Gradient Descent - Stopping Criterion

- ▶ The **cost function minimum** property: the **gradient** has to be **zero**.

$$\nabla_w J(\mathbf{w}) = 0$$





Gradient Descent - Descent Direction (1/2)

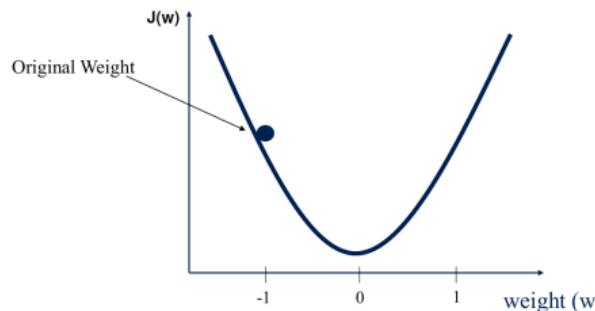
- ▶ Direction in which the **function value decreases** near the current point.
- ▶ Find the **direction of descent (slope)**.

Gradient Descent - Descent Direction (1/2)

- ▶ Direction in which the **function value decreases** near the current point.
- ▶ Find the **direction of descent (slope)**.
- ▶ Example:

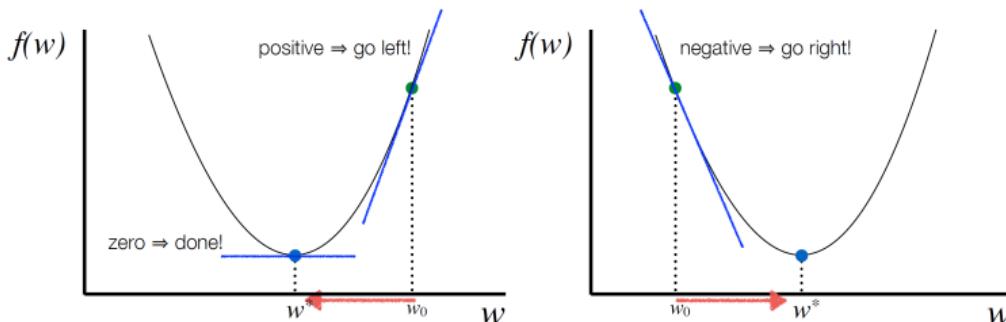
$$J(w) = w^2$$

$$\frac{\partial J(w)}{\partial w} = 2w = -2 \text{ at } w = -1$$



Gradient Descent - Descent Direction (2/2)

- Follow the opposite direction of the slope.



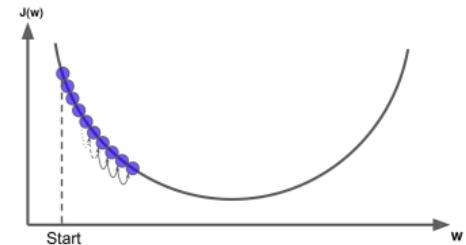


Gradient Descent - Learning Rate

- ▶ **Learning rate**: the length of steps.

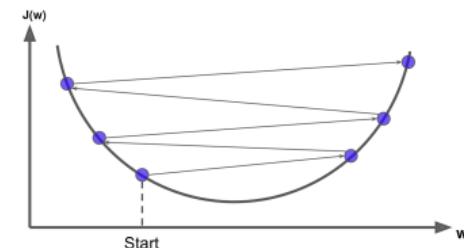
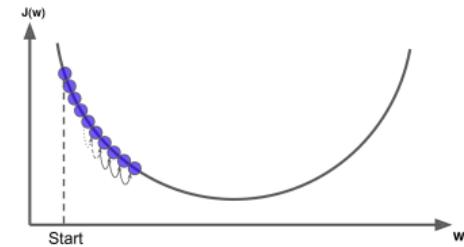
Gradient Descent - Learning Rate

- ▶ **Learning rate**: the length of steps.
- ▶ If it is **too small**: many iterations to converge.



Gradient Descent - Learning Rate

- ▶ **Learning rate**: the length of steps.
- ▶ If it is **too small**: many iterations to converge.
- ▶ If it is **too high**: the algorithm might diverge.



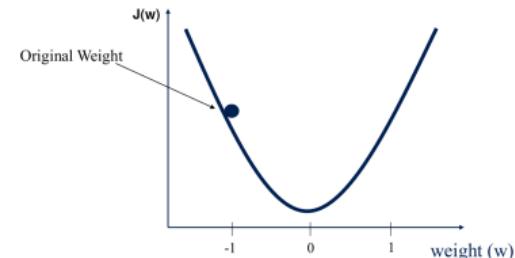


Gradient Descent - How to Learn Model Parameters w ?

- ▶ **Goal:** find w that minimizes $J(w) = \sum_{i=1}^m (w^T x^{(i)} - y^{(i)})^2$.

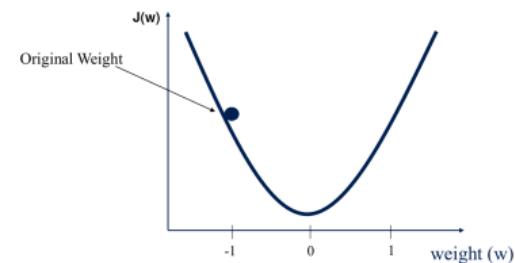
Gradient Descent - How to Learn Model Parameters w ?

- ▶ **Goal:** find w that minimizes $J(w) = \sum_{i=1}^m (w^T x^{(i)} - y^{(i)})^2$.
- ▶ Start at a **random point**, and repeat the following **steps**, until the **stopping criterion** is satisfied:



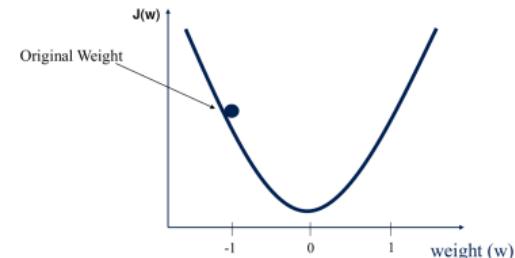
Gradient Descent - How to Learn Model Parameters w ?

- ▶ **Goal:** find w that minimizes $J(w) = \sum_{i=1}^m (w^T x^{(i)} - y^{(i)})^2$.
- ▶ Start at a **random point**, and repeat the following **steps**, until the **stopping criterion** is satisfied:
 1. Determine a **descent direction** $\frac{\partial J(w)}{\partial w}$



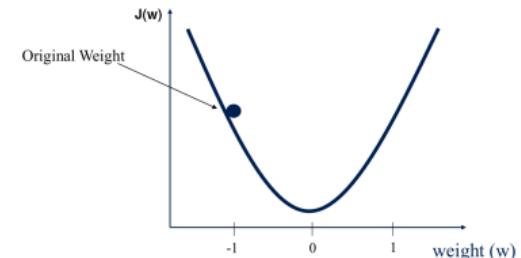
Gradient Descent - How to Learn Model Parameters w ?

- ▶ Goal: find w that minimizes $J(w) = \sum_{i=1}^m (w^T x^{(i)} - y^{(i)})^2$.
- ▶ Start at a random point, and repeat the following steps, until the stopping criterion is satisfied:
 1. Determine a descent direction $\frac{\partial J(w)}{\partial w}$
 2. Choose a step size η



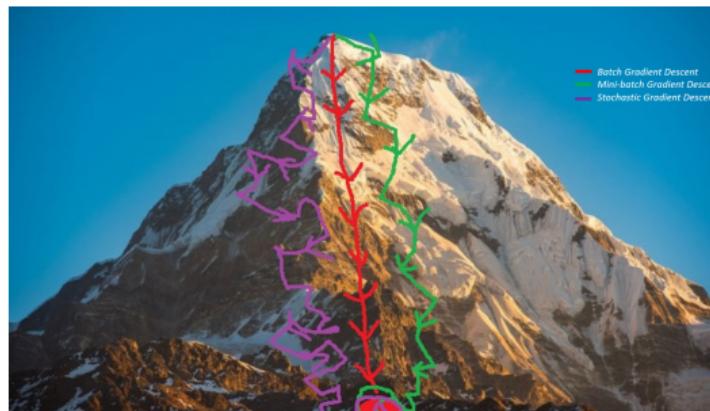
Gradient Descent - How to Learn Model Parameters w ?

- ▶ Goal: find w that minimizes $J(w) = \sum_{i=1}^m (w^T x^{(i)} - y^{(i)})^2$.
- ▶ Start at a random point, and repeat the following steps, until the stopping criterion is satisfied:
 1. Determine a descent direction $\frac{\partial J(w)}{\partial w}$
 2. Choose a step size η
 3. Update the parameters: $w^{(\text{next})} = w - \eta \frac{\partial J(w)}{\partial w}$
(should be done for all parameters simultaneously)



Gradient Descent - Different Algorithms

- ▶ Batch gradient descent
- ▶ Stochastic gradient descent
- ▶ Mini-batch gradient descent



[<https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3>]



Batch Gradient Descent



Batch Gradient Descent (1/2)

- ▶ Repeat the following **steps**, until the **stopping criterion** is satisfied:

1. Determine a **descent direction** $\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}$ for all parameters \mathbf{w} .

$$J(\mathbf{w}) = \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)})^2$$



Batch Gradient Descent (1/2)

- ▶ Repeat the following **steps**, until the stopping criterion is satisfied:

1. Determine a **descent direction** $\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}$ for all parameters \mathbf{w} .

$$J(\mathbf{w}) = \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)})^2$$

$$\frac{\partial J(\mathbf{w})}{\partial w_j} = \frac{2}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) x_j^{(i)}$$
$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \begin{bmatrix} \frac{\partial J(\mathbf{w})}{\partial w_0} \\ \frac{\partial J(\mathbf{w})}{\partial w_1} \\ \vdots \\ \frac{\partial J(\mathbf{w})}{\partial w_n} \end{bmatrix} = \frac{2}{m} \mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

2. Choose a **step size** η



Batch Gradient Descent (1/2)

- ▶ Repeat the following **steps**, until the stopping criterion is satisfied:

1. Determine a **descent direction** $\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}$ for all parameters \mathbf{w} .

$$J(\mathbf{w}) = \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)})^2$$

$$\frac{\partial J(\mathbf{w})}{\partial w_j} = \frac{2}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) x_j^{(i)}$$
$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \begin{bmatrix} \frac{\partial J(\mathbf{w})}{\partial w_0} \\ \frac{\partial J(\mathbf{w})}{\partial w_1} \\ \vdots \\ \frac{\partial J(\mathbf{w})}{\partial w_n} \end{bmatrix} = \frac{2}{m} \mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

2. Choose a **step size** η
3. **Update** the parameters: $\mathbf{w}^{(\text{next})} = \mathbf{w} - \eta \nabla_{\mathbf{w}} J(\mathbf{w})$



Batch Gradient Descent (2/2)

- ▶ The algorithm is called **Batch Gradient Descent**, because at each step, calculations are over the **full training set X** .
- ▶ As a result it is **slow on very large training sets**, i.e., large m .
- ▶ But, it **scales well** with the **number of features n** .

Batch Gradient Descent - Example (1/5)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2$$

$$\mathbf{X} = \left[\begin{array}{c|ccc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array} \right] \quad \mathbf{y} = \left[\begin{array}{c} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{array} \right]$$

Batch Gradient Descent - Example (2/5)

$$\mathbf{X} = \left[\begin{array}{c|ccc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array} \right] \quad \mathbf{y} = \left[\begin{array}{c} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{array} \right]$$

$$\begin{aligned}\frac{\partial J(\mathbf{w})}{\partial w_0} &= \frac{2}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) x_0^{(i)} \\ &= \frac{2}{5} [(w_0 + 2104w_1 + 3w_2 - 400) + (w_0 + 1600w_1 + 3w_2 - 330) + \\ &\quad (w_0 + 2400w_1 + 3w_2 - 369) + (w_0 + 1416w_1 + 2w_2 - 232) + (w_0 + 3000w_1 + 4w_2 - 540)]\end{aligned}$$

Batch Gradient Descent - Example (3/5)

$$\mathbf{X} = \left[\begin{array}{c|ccc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array} \right] \quad \mathbf{y} = \left[\begin{array}{c} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{array} \right]$$

$$\begin{aligned}
 \frac{\partial J(\mathbf{w})}{\partial w_1} &= \frac{2}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}_1^{(i)} \\
 &= \frac{2}{5} [2104(w_0 + 2104w_1 + 3w_2 - 400) + 1600(w_0 + 1600w_1 + 3w_2 - 330) + \\
 &\quad 2400(w_0 + 2400w_1 + 3w_2 - 369) + 1416(w_0 + 1416w_1 + 2w_2 - 232) + 3000(w_0 + 3000w_1 + 4w_2 - 540)]
 \end{aligned}$$

Batch Gradient Descent - Example (4/5)

$$\mathbf{X} = \left[\begin{array}{c|ccc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array} \right] \quad \mathbf{y} = \left[\begin{array}{c} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{array} \right]$$

$$\begin{aligned} \frac{\partial J(\mathbf{w})}{\partial w_2} &= \frac{2}{m} \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) x_2^{(i)} \\ &= \frac{2}{5} [3(w_0 + 2104w_1 + 3w_2 - 400) + 3(w_0 + 1600w_1 + 3w_2 - 330) + \\ &\quad 3(w_0 + 2400w_1 + 3w_2 - 369) + 2(w_0 + 1416w_1 + 2w_2 - 232) + 4(w_0 + 3000w_1 + 4w_2 - 540)] \end{aligned}$$



Batch Gradient Descent - Example (5/5)

$$w_0^{(\text{next})} = w_0 - \eta \frac{\partial J(w)}{\partial w_0}$$

$$w_1^{(\text{next})} = w_1 - \eta \frac{\partial J(w)}{\partial w_1}$$

$$w_2^{(\text{next})} = w_2 - \eta \frac{\partial J(w)}{\partial w_2}$$



Stochastic Gradient Descent



Stochastic Gradient Descent (1/3)

- ▶ Batch gradient descent problem: it's slow, because it uses the whole training set to compute the gradients at every step.

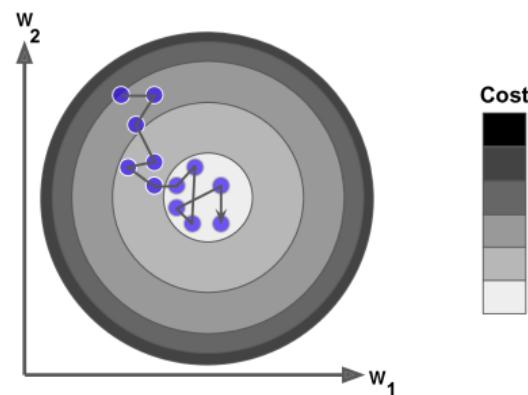


Stochastic Gradient Descent (1/3)

- ▶ **Batch gradient descent problem:** it's **slow**, because it uses the **whole training set** to compute the gradients at **every step**.
- ▶ **Stochastic gradient descent** computes the gradients based on only a **single instance**.
 - It picks a **random instance** in the **training set** at **every step**.

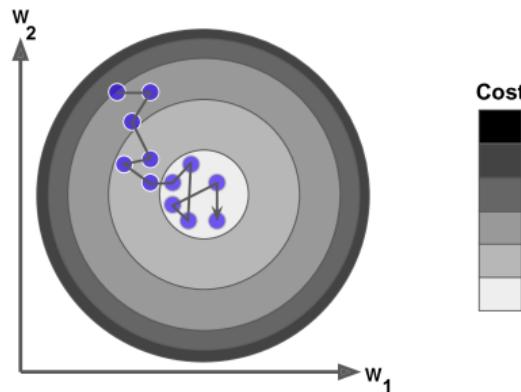
Stochastic Gradient Descent (2/3)

- ▶ The algorithm is much **faster**, but **less regular** than batch gradient descent.



Stochastic Gradient Descent (2/3)

- ▶ The algorithm is much **faster**, but **less regular** than batch gradient descent.
 - Instead of decreasing until it reaches the minimum, the **cost function will bounce up and down**.
 - It **never settles down**.





Stochastic Gradient Descent (3/3)

- ▶ With randomness the algorithm **can never settle at the minimum**.
- ▶ One solution is **simulated annealing**: start with **large learning rate**, then make it **smaller and smaller**.



Stochastic Gradient Descent (3/3)

- ▶ With randomness the algorithm **can never settle at the minimum**.
- ▶ One solution is **simulated annealing**: start with **large learning rate**, then make it **smaller and smaller**.
- ▶ **Learning schedule**: the function that **determines the learning rate** at each step.



Stochastic Gradient Descent - Example (1/3)

Living area	No. of bedrooms	Price
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2$$

$$\mathbf{X} = \left[\begin{array}{ccc|c} 1 & 2104 & 3 & 400 \\ 1 & 1600 & 3 & 330 \\ 1 & 2400 & 3 & 369 \\ 1 & 1416 & 2 & 232 \\ 1 & 3000 & 4 & 540 \end{array} \right] \quad \mathbf{y} = \left[\begin{array}{c} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{array} \right]$$

Stochastic Gradient Descent - Example (2/3)

$$\mathbf{X} = \left[\begin{array}{c|ccc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array} \right] \quad \mathbf{y} = \left[\begin{array}{c} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{array} \right]$$

$$\frac{\partial J(\mathbf{w})}{\partial w_0} = \frac{2}{m} (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) x_0^{(i)} = \frac{2}{5} [(w_0 + 1600w_1 + 3w_2 - 330)]$$

$$\frac{\partial J(\mathbf{w})}{\partial w_1} = \frac{2}{m} (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) x_1^{(i)} = \frac{2}{5} [1416(w_0 + 1416w_1 + 2w_2 - 232)]$$

$$\frac{\partial J(\mathbf{w})}{\partial w_2} = \frac{2}{m} (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}) x_2^{(i)} = \frac{2}{5} [3(w_0 + 2104w_1 + 3w_2 - 400)]$$



Stochastic Gradient Descent - Example (3/3)

$$w_0^{(\text{next})} = w_0 - \eta \frac{\partial J(w)}{\partial w_0}$$

$$w_1^{(\text{next})} = w_1 - \eta \frac{\partial J(w)}{\partial w_1}$$

$$w_2^{(\text{next})} = w_2 - \eta \frac{\partial J(w)}{\partial w_2}$$



Mini-Batch Gradient Descent

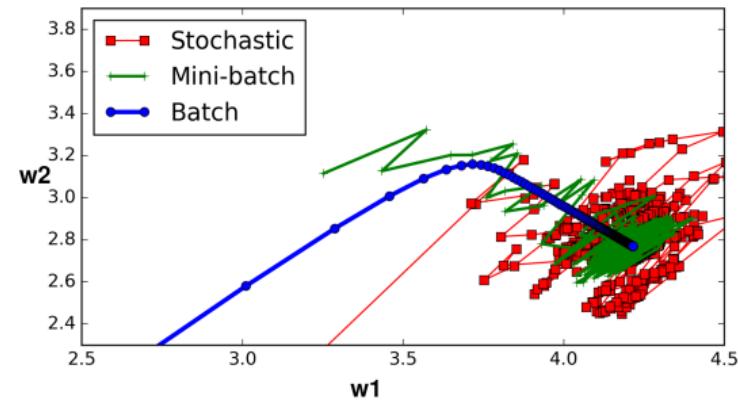


Mini-Batch Gradient Descent

- ▶ **Batch gradient descent**: at each step, it computes the gradients based on the **full training set**.
- ▶ **Stochastic gradient descent**: at each step, it computes the gradients based on **just one instance**.
- ▶ **Mini-batch gradient descent**: at each step, it computes the gradients based on small **random sets of instances** called **mini-batches**.

Comparison of Algorithms for Linear Regression

Algorithm	Large m	Large n
Normal Equation	Fast	Slow
Batch GD	Slow	Fast
Stochastic GD	Fast	Fast
Mini-batch GD	Fast	Fast





Gradient Descent in Spark

```
val data = spark.read.format("libsvm").load("data.txt")
```



Gradient Descent in Spark

```
val data = spark.read.format("libsvm").load("data.txt")
```

```
import org.apache.spark.ml.regression.LinearRegression
```

```
val lr = new LinearRegression().setMaxIter(10)
```

```
val lrModel = lr.fit(data)
```



Gradient Descent in Spark

```
val data = spark.read.format("libsvm").load("data.txt")

import org.apache.spark.ml.regression.LinearRegression

val lr = new LinearRegression().setMaxIter(10)

val lrModel = lr.fit(data)

println(s"Coefficients: ${lrModel.coefficients} Intercept: ${lrModel.intercept}")

val trainingSummary = lrModel.summary
println(s"RMSE: ${trainingSummary.rootMeanSquaredError}")
```



Generalization



Training Data and Test Data

- ▶ Split data into a **training set** and a **test set**.

```
val data = spark.read.format("libsvm").load("data.txt")  
  
val Array(trainDF, testDF) = data.randomSplit(Array(0.8, 0.2))
```

Full Dataset:

Training Data	Test Data
---------------	-----------



Training Data and Test Data

- ▶ Split data into a **training set** and a **test set**.
- ▶ Use **training set** when **training a machine learning model**.
 - Compute **training error** on the training set.
 - Try to **reduce** this training error.

```
val data = spark.read.format("libsvm").load("data.txt")  
  
val Array(trainDF, testDF) = data.randomSplit(Array(0.8, 0.2))
```

Full Dataset:

Training Data	Test Data
---------------	-----------



Training Data and Test Data

- ▶ Split data into a **training set** and a **test set**.
- ▶ Use **training set** when **training a machine learning model**.
 - Compute **training error** on the training set.
 - Try to **reduce** this training error.
- ▶ Use **test set** to **measure the accuracy of the model**.
 - **Test error** is the error when you run the **trained model** on **test data (new data)**.

```
val data = spark.read.format("libsvm").load("data.txt")  
  
val Array(trainDF, testDF) = data.randomSplit(Array(0.8, 0.2))
```

Full Dataset:

Training Data	Test Data
---------------	-----------



Generalization

- ▶ **Generalization:** make a model that performs **well** on **test data**.
 - Have a **small test error**.



Generalization

- ▶ **Generalization:** make a model that performs **well** on **test data**.
 - Have a **small test error**.
- ▶ **Challenges**
 1. Make the **training error small**.
 2. Make the **gap** between **training** and **test error small**.



More About The Test Error

- ▶ The **test error** is defined as the **expected value** of the **error** on test set.

$$\begin{aligned} \text{MSE} &= \frac{1}{k} \sum_i^k (\hat{y}^{(i)} - y^{(i)})^2, \quad k: \text{the num. of instances in the test set} \\ &= E[(\hat{y} - y)^2] \end{aligned}$$



More About The Test Error

- ▶ The **test error** is defined as the **expected value** of the **error** on test set.

$$\begin{aligned} \text{MSE} &= \frac{1}{k} \sum_i^k (\hat{y}^{(i)} - y^{(i)})^2, \quad k: \text{the num. of instances in the test set} \\ &= E[(\hat{y} - y)^2] \end{aligned}$$

- ▶ A model's **test error** can be expressed as the **sum** of **bias** and **variance**.

$$E[(\hat{y} - y)^2] = \text{Bias}[\hat{y}, y]^2 + \text{Var}[\hat{y}] + \varepsilon^2$$



Bias and Underfitting

- ▶ **Bias**: the expected **deviation** from the **true value** of the function.
 - Bias is the same as the **mean squared error**.

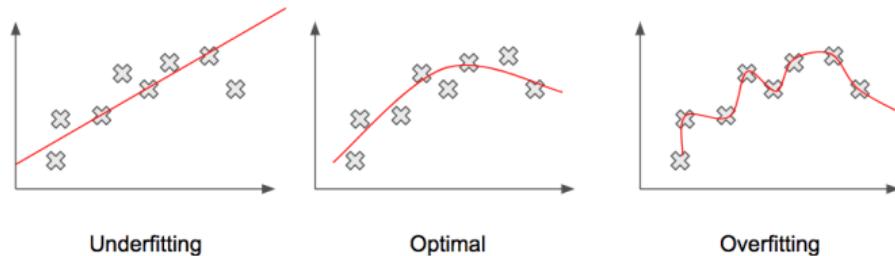
$$\text{Bias}[\hat{y}, y] = E[(\hat{y} - y)^2]$$

Bias and Underfitting

- ▶ **Bias**: the expected **deviation** from the **true value** of the function.
 - Bias is the same as the **mean squared error**.

$$\text{Bias}[\hat{y}, y] = E[(\hat{y} - y)^2]$$

- ▶ A **high-bias** model is most likely to **underfit** the training data.
 - High **error** value on the **training set**.

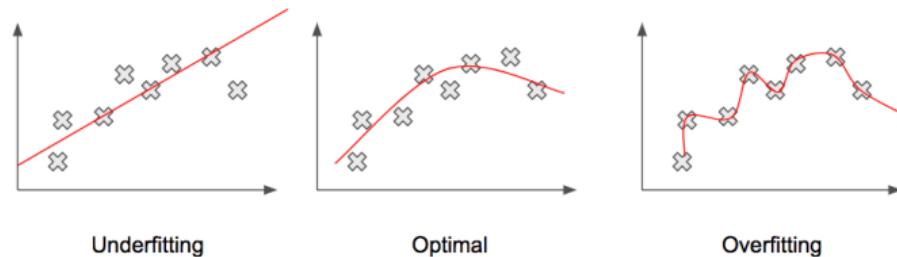


Bias and Underfitting

- ▶ **Bias**: the expected **deviation** from the **true value** of the function.
 - Bias is the same as the **mean squared error**.

$$\text{Bias}[\hat{y}, y] = E[(\hat{y} - y)^2]$$

- ▶ A **high-bias** model is most likely to **underfit** the training data.
 - **High error** value on the **training set**.
- ▶ **Underfitting** happens when the **model is too simple** to learn the underlying structure of the data.





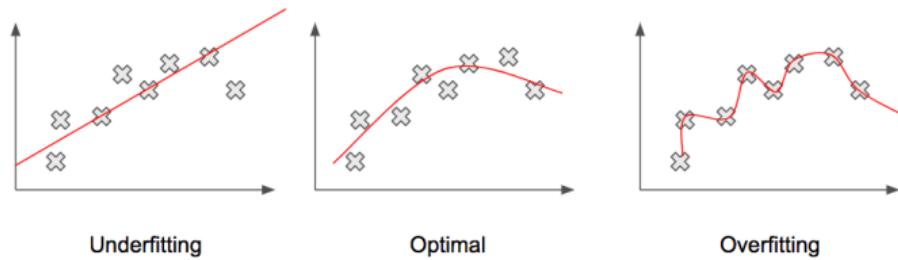
Variance and Overfitting

- ▶ **Variance**: how much a model **changes** if you train it on a different training set.

$$\text{Var}[\hat{y}] = E[(\hat{y} - E[\hat{y}])^2]$$

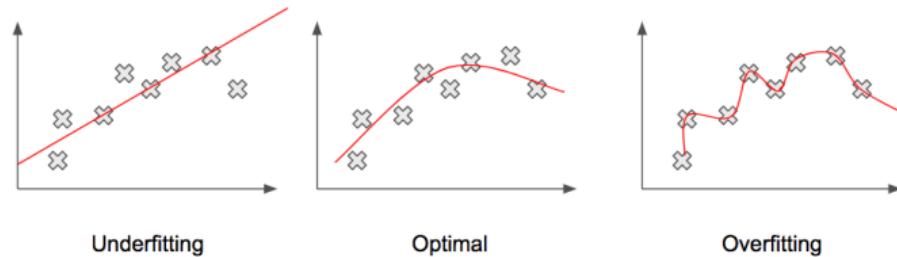
Variance and Overfitting

- ▶ **Variance:** how much a model changes if you train it on a different training set.
$$\text{Var}[\hat{y}] = E[(\hat{y} - E[\hat{y}])^2]$$
- ▶ A **high-variance** model is most likely to **overfit** the training data.
 - The **gap** between the **training error** and **test error** is **too large**.



Variance and Overfitting

- ▶ **Variance**: how much a model changes if you train it on a different training set.
$$\text{Var}[\hat{y}] = E[(\hat{y} - E[\hat{y}])^2]$$
- ▶ A **high-variance** model is most likely to **overfit** the training data.
 - The **gap** between the **training error** and **test error** is **too large**.
- ▶ **Overfitting** happens when the **model is too complex** relative to the amount and noisiness of the training data.





The Bias/Variance Tradeoff (1/2)

- ▶ Assume a model with two parameters w_0 (intercept) and w_1 (slope): $\hat{y} = w_0 + w_1 x$



The Bias/Variance Tradeoff (1/2)

- ▶ Assume a model with **two parameters** w_0 (**intercept**) and w_1 (**slope**): $\hat{y} = w_0 + w_1 x$
- ▶ They give the learning algorithm **two degrees of freedom**.



The Bias/Variance Tradeoff (1/2)

- ▶ Assume a model with two parameters w_0 (intercept) and w_1 (slope): $\hat{y} = w_0 + w_1 x$
- ▶ They give the learning algorithm two degrees of freedom.
- ▶ We tweak both the w_0 and w_1 to adapt the model to the training data.

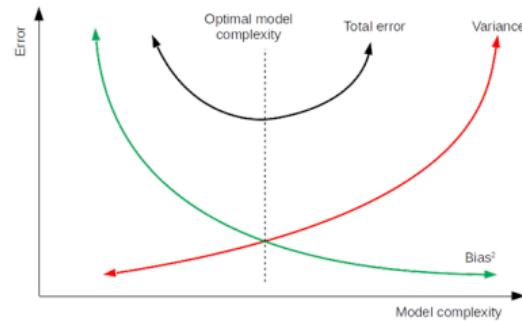
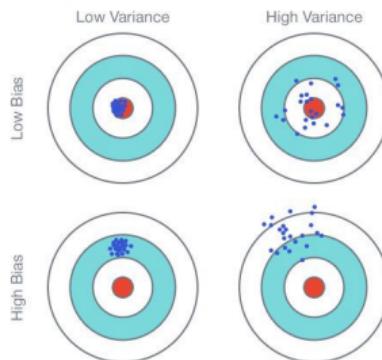


The Bias/Variance Tradeoff (1/2)

- ▶ Assume a model with two parameters w_0 (intercept) and w_1 (slope): $\hat{y} = w_0 + w_1 x$
- ▶ They give the learning algorithm two degrees of freedom.
- ▶ We tweak both the w_0 and w_1 to adapt the model to the training data.
- ▶ If we forced $w_0 = 0$, the algorithm would have only one degree of freedom and would have a much harder time fitting the data properly.

The Bias/Variance Tradeoff (2/2)

- ▶ Increasing degrees of freedom will typically increase its variance and reduce its bias.
- ▶ Decreasing degrees of freedom increases its bias and reduces its variance.
- ▶ This is why it is called a **tradeoff**.





Regularization (1/2)

- ▶ One way to reduce the risk of overfitting is to have fewer degrees of freedom.
- ▶ Regularization is a technique to reduce the risk of overfitting.
- ▶ For a linear model, regularization is achieved by constraining the weights of the model.

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) + \lambda R(\mathbf{w})$$



Regularization (2/2)

- ▶ Lasso regression (1): $R(\mathbf{w}) = \lambda \sum_{i=1}^n |w_i|$ is added to the cost function:

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) + \lambda \sum_{i=1}^n |w_i|$$



Regularization (2/2)

- ▶ Lasso regression (1): $R(\mathbf{w}) = \lambda \sum_{i=1}^n |w_i|$ is added to the cost function:

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) + \lambda \sum_{i=1}^n |w_i|$$

- ▶ Ridge regression (2): $R(\mathbf{w}) = \lambda \sum_{i=1}^n w_i^2$ is added to the cost function.

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) + \lambda \sum_{i=1}^n w_i^2$$



Regularization (2/2)

- ▶ Lasso regression (/1): $R(\mathbf{w}) = \lambda \sum_{i=1}^n |w_i|$ is added to the cost function:

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) + \lambda \sum_{i=1}^n |w_i|$$

- ▶ Ridge regression (/2): $R(\mathbf{w}) = \lambda \sum_{i=1}^n w_i^2$ is added to the cost function.

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) + \lambda \sum_{i=1}^n w_i^2$$

- ▶ ElasticNet: a middle ground between /1 and /2 regularization.

$$J(\mathbf{w}) = \text{MSE}(\mathbf{w}) + \alpha \lambda \sum_{i=1}^n |w_i| + (1 - \alpha) \lambda \sum_{i=1}^n w_i^2$$



Regularization in Spark

$$J(w) = \text{MSE}(w) + \alpha \lambda \sum_{i=1}^n |w_i| + (1 - \alpha) \lambda \sum_{i=1}^n w_i^2$$

- ▶ If $\alpha = 0$: L_2 regularization
- ▶ If $\alpha = 1$: L_1 regularization
- ▶ For α in $(0, 1)$: a combination of L_1 and L_2 regularizations

```
import org.apache.spark.ml.regression.LinearRegression

val lr = new LinearRegression().setElasticNetParam(0.8)

val lrModel = lr.fit(data)
```



Hyperparameters



Hyperparameters and Validation Sets (1/2)

- ▶ Hyperparameters are settings that we can use to control the behavior of a learning algorithm.



Hyperparameters and Validation Sets (1/2)

- ▶ Hyperparameters are settings that we can use to control the behavior of a learning algorithm.
- ▶ The values of hyperparameters are not adapted by the learning algorithm itself.
 - E.g., the α and λ values for regularization.



Hyperparameters and Validation Sets (1/2)

- ▶ Hyperparameters are settings that we can use to control the behavior of a learning algorithm.
- ▶ The values of hyperparameters are not adapted by the learning algorithm itself.
 - E.g., the α and λ values for regularization.
- ▶ We do not learn the hyperparameter.
 - It is not appropriate to learn that hyperparameter on the training set.
 - If learned on the training set, such hyperparameters would always result in overfitting.



Hyperparameters and Validation Sets (2/2)

- ▶ To find **hyperparameters**, we need a **validation set** of examples that the **training algorithm does not observe**.



Hyperparameters and Validation Sets (2/2)

- ▶ To find **hyperparameters**, we need a **validation set** of examples that the **training algorithm does not observe**.
- ▶ We construct the **validation set** from the **training data** (**not the test data**).



Hyperparameters and Validation Sets (2/2)

- ▶ To find **hyperparameters**, we need a **validation set** of examples that the **training algorithm does not observe**.
- ▶ We construct the **validation set** from the **training data** (**not the test data**).
- ▶ We split the **training data** into two disjoint subsets:
 1. One is used to **learn the parameters**.
 2. The other one (the **validation set**) is used to **estimate the test error** **during or after training**, allowing for the **hyperparameters** to be updated accordingly.

Full Dataset:

Training Data	Validation Data	Test Data

Cross-Validation

- ▶ **Cross-validation:** a technique to avoid **wasting too much training data in validation sets.**



Cross-Validation

- ▶ **Cross-validation:** a technique to avoid **wasting too much training data** in **validation sets**.
- ▶ The **training set** is split into **complementary subsets**.



Cross-Validation

- ▶ **Cross-validation:** a technique to avoid **wasting too much training data** in **validation sets**.
- ▶ The **training set** is split into **complementary subsets**.
- ▶ Each model is **trained** against a different **combination** of these subsets and **validated** against the **remaining parts**.



Cross-Validation

- ▶ **Cross-validation:** a technique to avoid **wasting too much training data** in **validation sets**.
- ▶ The **training set** is split into **complementary subsets**.
- ▶ Each model is **trained** against a different **combination** of these subsets and **validated** against the **remaining parts**.
- ▶ Once the model type and hyperparameters have been selected, a **final model** is trained using these hyperparameters on the **full training set**, and the test error is measured on the **test set**.





Hyperparameters and Cross-Validation in Spark (1/2)

- ▶ **CrossValidator** to optimize hyperparameters in algorithms and model selection.
- ▶ It requires the following items:
 - **Estimator**: algorithm or Pipeline to tune.
 - Set of **ParamMaps**: parameters to choose from (also called a **parameter grid**).
 - **Evaluator**: metric to measure **how well a fitted Model does on held-out test data**.



Hyperparameters and Cross-Validation in Spark (2/2)

```
// construct a grid of parameters to search over.  
// this grid has 2 x 2 = 4 parameter settings for CrossValidator to choose from.  
val paramGrid = new ParamGridBuilder()  
  .addGrid(lr.regParam, Array(0.1, 0.01))  
  .addGrid(lr.elasticNetParam, Array(0.0, 1.0))  
  .build()
```



Hyperparameters and Cross-Validation in Spark (2/2)

```
// construct a grid of parameters to search over.  
// this grid has 2 x 2 = 4 parameter settings for CrossValidator to choose from.  
val paramGrid = new ParamGridBuilder()  
  .addGrid(lr.regParam, Array(0.1, 0.01))  
  .addGrid(lr.elasticNetParam, Array(0.0, 1.0))  
  .build()
```

```
val lr = new LinearRegression()  
  
// num folds = 3 => (2 x 2) x 3 = 12 different models being trained  
val cv = new CrossValidator()  
  .setEstimator(lr)  
  .setEvaluator(new RegressionEvaluator())  
  .setEstimatorParamMaps(paramGrid)  
  .setNumFolds(3)  
  
val cvModel = cv.fit(trainDF)
```



Summary

Summary

- ▶ Linear regression model $\hat{y} = \mathbf{w}^T \mathbf{x}$
 - Learning parameters \mathbf{w}
 - Cost function $J(\mathbf{w})$
 - Learn parameters: normal equation, gradient descent (batch, stochastic, mini-batch)
- ▶ Generalization
 - Overfitting vs. underfitting
 - Bias vs. variance
 - Regularization: Lasso regression, Ridge regression, ElasticNet
- ▶ Hyperparameters and cross-validation



Reference

- ▶ Ian Goodfellow et al., Deep Learning (Ch. 4, 5)
- ▶ Aurélien Géron, Hands-On Machine Learning (Ch. 2, 4)
- ▶ Matei Zaharia et al., Spark - The Definitive Guide (Ch. 27)



Questions?